

chain nodes :

7 20

ring nodes :

1 2 3 4 5 6 8 9 10 11 12 13 14 15 16

chain bonds :

6-7 7-8 9-20

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12 11-13 12-16 13-14 14-15  
15-16

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-20

exact bonds :

6-7 7-8 9-10 10-11

normalized bonds :

11-12 11-13 12-16 13-14 14-15 15-16

isolated ring systems :

containing 1 : 8 :

G1:O,S

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 20:CLASS

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 "Ask CAS" for self-help around the clock  
NEWS 3 NOV 24 MSDS-CCOHS file reloaded  
NEWS 4 DEC 08 CABA reloaded with left truncation  
NEWS 5 DEC 08 IMS file names changed  
NEWS 6 DEC 17 DGENE: Two new display fields added  
NEWS 7 DEC 18 BIOTECHNO no longer updated  
NEWS 8 DEC 19 CROPU no longer updated; subscriber discount no longer available  
NEWS 9 DEC 22 ABI-INFORM now available on STN  
NEWS 10 JAN 27 Source of Registration (SR) information in REGISTRY updated and searchable  
NEWS 11 JAN 27 A new search aid, the Company Name Thesaurus, available in CA/CAPLUS  
NEWS 12 FEB 05 German (DE) application and patent publication number format changes  
NEWS 13 MAR 03 MEDLINE and LMEADLINE reloaded  
NEWS 14 MAR 03 MEDLINE file segment of TOXCENTER reloaded  
NEWS 15 MAR 03 FRANCEPAT now available on STN  
NEWS 16 MAR 29 Pharmaceutical Substances (PS) now available on STN  
NEWS 17 MAR 29 WPIFV now available on STN  
NEWS 18 MAR 29 No connect hour charges in WPIFV until May 1, 2004  
NEWS 19 MAR 29 New monthly current-awareness alert (SDI) frequency in RAPRA  
  
NEWS EXPRESS MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 3 MARCH 2004  
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FILE 'HOME' ENTERED AT 15:22:35 ON 09 APR 2004

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 15:22:40 ON 09 APR 2004

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STRUCTURE FILE UPDATES: 7 APR 2004 HIGHEST RN 672883-15-7  
DICTIONARY FILE UPDATES: 7 APR 2004 HIGHEST RN 672883-15-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

L1 STRUCTURE UPLOADED

=> l1

L1 IS NOT A RECOGNIZED COMMAND

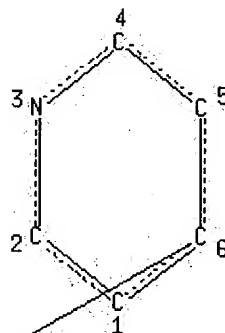
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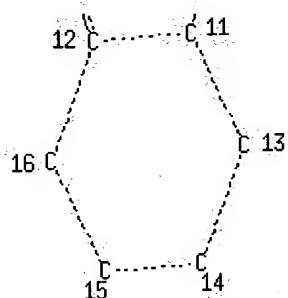
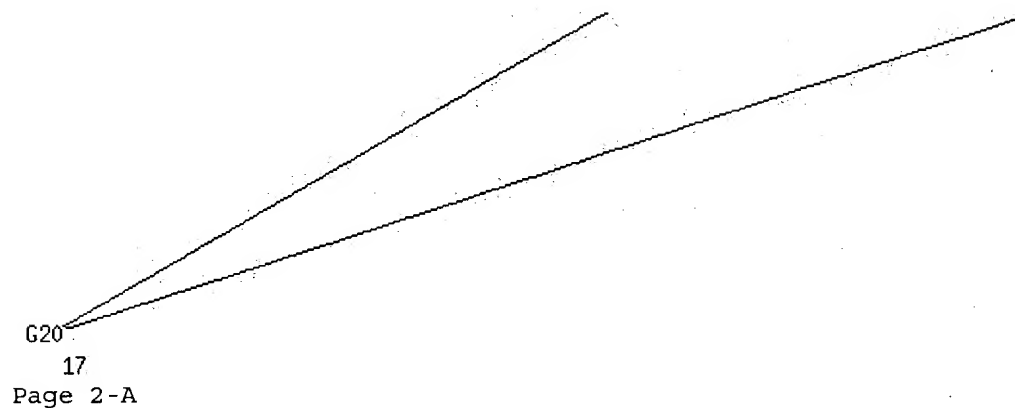
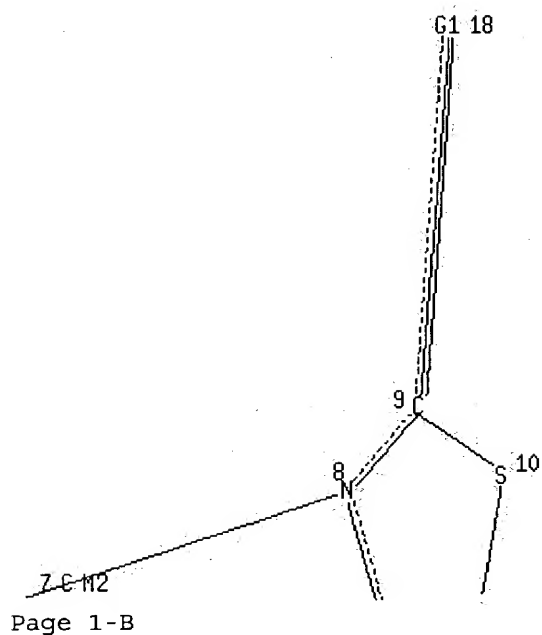
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L1 HAS NO ANSWERS

L1 STR

0 19 S 20





Page 2-B  
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 REP G20=(1-2) 7-6 7-8  
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NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS C	AT	7
NSPEC	IS R	AT	8
NSPEC	IS R	AT	9

NSPEC IS R AT 10  
 NSPEC IS R AT 11  
 NSPEC IS R AT 12  
 NSPEC IS R AT 13  
 NSPEC IS R AT 14  
 NSPEC IS R AT 15  
 NSPEC IS R AT 16  
 NSPEC IS C AT 17  
 NSPEC IS C AT 18  
 DEFAULT MLEVEL IS ATOM  
 MLEVEL IS CLASS AT 7 19 20  
 DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RSPEC I  
 NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

=> s 11

SAMPLE SEARCH INITIATED 15:25:32 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 5 TO ITERATE

100.0% PROCESSED 5 ITERATIONS 2 ANSWERS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 5 TO 234  
 PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> s 11 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS  
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
 FULL SEARCH INITIATED 15:25:36 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 104 TO ITERATE

100.0% PROCESSED 104 ITERATIONS 45 ANSWERS  
 SEARCH TIME: 00.00.01

L3 45 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	157.10	157.31

FILE 'HCAPLUS' ENTERED AT 15:25:39 ON 09 APR 2004  
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FILE COVERS 1907 - 9 Apr 2004 VOL 140 ISS 16  
FILE LAST UPDATED: 8 Apr 2004 (20040408/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L4 7 L3

=> s 14 and rocher, j?/au

69 ROCHER, J?/AU

L5 1 L4 AND ROCHER, J?/AU

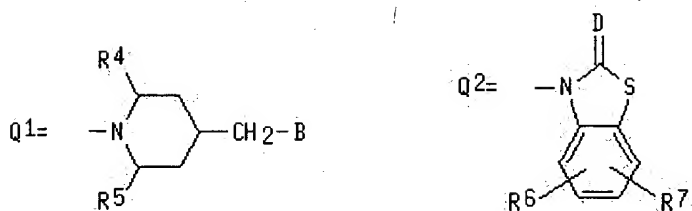
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L5 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 1999:311193 HCAPLUS  
DOCUMENT NUMBER: 130:338102  
TITLE: Preparation of N-(aminoalkyl)- or N-(1-piperidinylmethyl)benzothiazoline derivatives as ligands for sigma-receptor  
INVENTOR(S): **Rocher, Jean-Philippe**; Yamabe, Haruko; Chaki, Haruyuki; Saito, Ken-ichi; Abe, Michikazu; Okuyama, Masahiro  
PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan  
SOURCE: PCT Int. Appl., 95 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9923083	A1	19990514	WO 1998-JP4973	19981104
W: CA, CN, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1043319	A1	20001011	EP 1998-951687	19981104
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 11217377	A2	19990810	JP 1998-314459	19981105
PRIORITY APPLN. INFO.:			JP 1997-302607	A 19971105
			WO 1998-JP4973	W 19981104
OTHER SOURCE(S):		MARPAT 130:338102		
GI				



AB Compds. represented by the following formula, such as (R,S)-1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol, or salts thereof: X-Q-C(R1)(R2)-Z [wherein R1 and R2 each represents hydrogen, alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; and Z represents either of groups NR<sub>3</sub>(CH<sub>2</sub>)<sub>p</sub> and Q1; wherein R<sub>3</sub> represents alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; p is an integer of 3 to 8; R<sub>4</sub> and R<sub>5</sub> each represents hydrogen or alkyl or they together with other interposing atoms represent a 5- to 7-membered heterocyclic ring; and B represents formula Q2 (wherein R<sub>6</sub> and R<sub>7</sub> each represents hydrogen, halogeno, NO<sub>2</sub>, alkyl, cycloalkyl, alkenyl, haloalkyl, OH, alkoxy, haloalkoxy, alkoxy-carbonyl, Ph, (un)substituted NH<sub>2</sub>, alkylthio, etc.); D represents sulfur, oxygen, or (un)substituted NH; when X represents optionally alkyl-substituted mono- or polycyclic alkyl, cycloalkylalkyl, aryl, or heteroaryl, Q represents CO, C(:NOH), C(Y)(A) (wherein Y represents H, alkyl, alkenyl, alkynyl, etc. and A represent OH, alkoxy, cycloalkoxy, cycloalkylalkoxy, alkenyloxy, aryloxy, etc.); or when X represents a 8- to 10-membered bicyclic heteroaryl contg. 1 or 2 heteroatoms, Q represents single bond], which have high affinity to  $\sigma$ -receptors and exhibit small inhibition consts. K<sub>i</sub> against  $\sigma$ -1 and/or  $\sigma$ -2 receptors, are prepd. Also claimed are therapeutics contg. I as the active ingredients for the treatment and/or prevention of diseases caused or enhanced by nerve-regulating effect of  $\sigma$ -ligands. They are useful for the treatment and/or prevention of central nervous system diseases, intestinal diseases, and cardiovascular diseases. Thus, 4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidine was condensed with 1-(bromoacetyl)adamantane in the presence of K<sub>2</sub>CO<sub>3</sub> followed by NaBH<sub>4</sub> redn. in ethanol and THF and acidification with HCl in EtOAc to give 1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol hydrochloride (II). II and 3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-5-chloro-2-oxobenzothiazoline hydrochloride inhibited the binding of [<sup>3</sup>H]-di-o-tolylguanidine to  $\sigma$ -receptor (P2 membrane fraction) prepn. from rat liver with K<sub>i</sub> value of 7.0 and 3.1 nM, resp., as compared to K<sub>i</sub> of 29 nM for haloperidol. A tablet, an injection, and an ointment formulation contg. II were described.

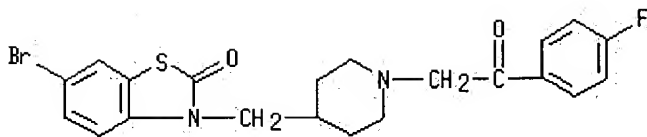
IT 224443-05-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of N-(aminoalkyl)- or N-(1-piperidinyl)benzothiazoline derivs. having high affinity to sigma-receptor as therapeutics)

RN 224443-05-4 HCAPLUS

CN 2(3H)-Benzothiazolone, 6-bromo-3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



# HCl

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=&gt; d his

(FILE 'HOME' ENTERED AT 15:22:35 ON 09 APR 2004)

FILE 'REGISTRY' ENTERED AT 15:22:40 ON 09 APR 2004

L1 STRUCTURE UPLOADED

L2 2 S L1

L3 45 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 15:25:39 ON 09 APR 2004

L4 7 S L3

L5 1 S L4 AND ROCHER, J?/AU

=&gt; s 14 and yamabe, h?/au

208 YAMABE, H?/AU

L6 1 L4 AND YAMABE, H?/AU

=&gt; s 16 not 15

L7 0 L6 NOT L5

=&gt; s 14 and chaki, h?/au

74 CHAKI, H?/AU

L8 1 L4 AND CHAKI, H?/AU

=&gt; s 18 not 16

L9 0 L8 NOT L6

=&gt; s 14 and abe, m?/au

5404 ABE, M?/AU

L10 1 L4 AND ABE, M?/AU

=&gt; s 110 not 16

L11 0 L10 NOT L6

=&gt; s 14 and okuyama, m?/au

959 OKUYAMA, M?/AU

L12 1 L4 AND OKUYAMA, M?/AU

=&gt; s 112 not 110

L13 0 L12 NOT L10

=&gt; d 14, ibib abs fhitr 1-7

L4 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

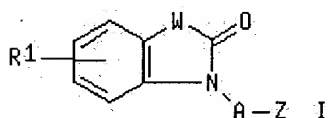
Full Text	Citing References
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ACCESSION NUMBER: 2001:372159 HCAPLUS

DOCUMENT NUMBER: 134:366868  
 TITLE: Preparation of benzothiazolines as neuropeptide Y receptor antagonists  
 INVENTOR(S): Sato, Yoshiya; Itani, Hiromichi; Tabuchi, Seiichiro; Sakata, Yoshihiko; Ohashi, Hiroko  
 PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 88 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001139574	A2	20010522	JP 2000-296175	20000928
PRIORITY APPLN. INFO.: AU 1999-3093			A	19990928
OTHER SOURCE(S): MARPAT 134:366868				

GI



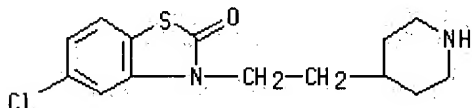
AB The title compds. I [R1 = H, halo; W = S, O; A = (CH2)n, etc.; n = 1 - 6; Z = (un)substituted N-contg. heterocyclic ring] are prepd.  
 1-[(5-Chloro-2-oxobenzothiazolin-3-yl)acetyl]piperidine-4-carboxylic acid  
 4-benzoylanilide showed IC100 of 10<sup>-7</sup> M in a neuropeptide Y5 receptor binding assay.

IT **340179-40-0P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (prepn. of benzothiazolines as neuropeptide Y receptor antagonists)

RN 340179-40-0 HCAPLUS

CN 2(3H)-Benzothiazolone, 5-chloro-3-[2-(4-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing  
 Text References

ACCESSION NUMBER: 1999:311193 HCAPLUS

DOCUMENT NUMBER: 130:338102

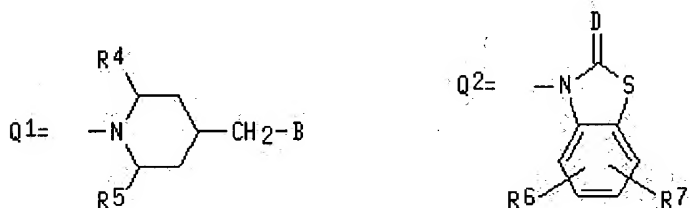
TITLE: Preparation of N-(aminoalkyl)- or N-(1-piperidinylmethyl)benzothiazoline derivatives as ligands for sigma-receptor

INVENTOR(S): Rocher, Jean-Philippe; Yamabe, Haruko; Chaki, Haruyuki; Saito, Ken-ichi; Abe, Michikazu; Okuyama, Masahiro

PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan

SOURCE: PCT Int. Appl., 95 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9923083	A1	19990514	WO 1998-JP4973	19981104
W: CA, CN, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1043319	A1	20001011	EP 1998-951687	19981104
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 11217377	A2	19990810	JP 1998-314459	19981105
PRIORITY APPLN. INFO.:			JP 1997-302607	A 19971105
			WO 1998-JP4973	W 19981104
OTHER SOURCE(S):		MARPAT 130:338102		
GI				



AB Compds. represented by the following formula, such as (R,S)-1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol, or salts thereof: X-Q-C(R1)(R2)-Z [wherein R1 and R2 each represents hydrogen, alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; and Z represents either of groups NR3(CH2)p and Q1; wherein R3 represents alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; p is an integer of 3 to 8; R4 and R5 each represents hydrogen or alkyl or they together with other interposing atoms represent a 5- to 7-membered heterocyclic ring; and B represents formula Q2 (wherein R6 and R7 each represents hydrogen, halogeno, NO2, alkyl, cycloalkyl, alkenyl, haloalkyl, OH, alkoxy, haloalkoxy, alkoxycarbonyl, Ph, (un)substituted NH2, alkylthio, etc.); D represents sulfur, oxygen, or (un)substituted NH; when X represents optionally alkyl-substituted mono- or polycyclic alkyl, cycloalkylalkyl, aryl, or heteroaryl, Q represents CO, C(:NOH), C(Y)(A) (wherein Y represents H, alkyl, alkenyl, alkynyl, etc. and A represents OH, alkoxy, cycloalkoxy, cycloalkylalkoxy, alkenyloxy, aryloxy, etc.); or when X represents a 8- to 10-membered bicyclic heteroaryl contg. 1 or 2 heteroatoms, Q represents single bond], which have high affinity to  $\sigma$ -receptors and exhibit small inhibition consts.  $K_i$  against  $\sigma$ -1 and/or  $\sigma$ -2 receptors, are prepd. Also claimed are therapeutics contg. I as the active ingredients for the treatment and/or prevention of diseases caused or enhanced by nerve-regulating effect of  $\sigma$ -ligands. They are useful for the treatment and/or prevention of central nervous system diseases, intestinal diseases, and cardiovascular diseases. Thus, 4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidine was condensed with 1-(bromoacetyl)adamantane in the presence of K2CO3 followed by NaBH4 redn. in ethanol and THF and acidification with HCl in EtOAc to give 1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-

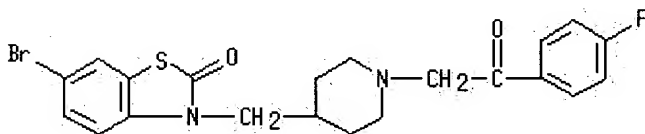
1-yl]ethanol hydrochloride (II). II and 3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-5-chloro-2-oxobenzothiazoline hydrochloride inhibited the binding of [H3]-di-o-tolylguanidine to  $\sigma$ -receptor (P2 membrane fraction) prepn. from rat liver with  $K_i$  value of 7.0 and 3.1 nM, resp., as compared to  $K_i$  of 29 nM for haloperidol. A tablet, an injection, and an ointment formulation contg. II were described.

IT 224443-05-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of N-(aminoalkyl)- or N-(1-piperidinyl)benzothiazoline derivs. having high affinity to sigma-receptor as therapeutics)

RN 224443-05-4 HCAPLUS

CN 2(3H)-Benzothiazolone, 6-bromo-3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



# HCl

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

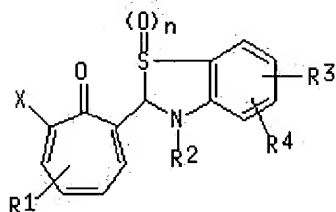
Full Text Citing References

ACCESSION NUMBER: 1993:191730 HCAPLUS  
DOCUMENT NUMBER: 118:191730  
TITLE: Preparation of benzothiazolinyltropolones for treatment of ischemia.  
INVENTOR(S): McWhoster, William W.; Ito, Noriie; Ozawa, Kazunori; Kushida, Hiroshi; Nomura, Toshiharu; Kuniyara, Mineo  
PATENT ASSIGNEE(S): Upjohn Co., USA  
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 3  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04247077	A2	19920903	JP 1991-56252	19910131
CA 2087004	AA	19920301	CA 1991-2087004	19910827
CA 2087004	C	19980421		
EP 546102	A1	19930616	EP 1991-917948	19910827
EP 546102	B1	19971015		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
HU 65943	A2	19940829	HU 1993-533	19910827
JP 06509318	T2	19941020	JP 1991-516629	19910827
JP 2512656	B2	19960703		
AT 159251	E	19971115	AT 1991-917948	19910827
ES 2109276	T3	19980116	ES 1991-917948	19910827

NO 9300669	A	19930225	NO 1993-669	19930225
US 5594144	A	19970114	US 1995-442710	19950518
US 5703071	A	19971230	US 1995-443972	19950518
PRIORITY APPLN. INFO.:			JP 1990-229536	19900829
			JP 1991-56252	19910131
			JP 1991-39173	19910208
			WO 1991-US5906	19910827
			US 1993-975924	19930218

OTHER SOURCE(S): MARPAT 118:191730  
GI



I

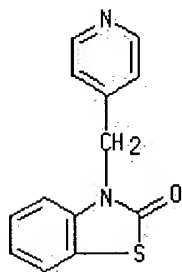
AB The title compds. [I; R1 = H, alkyl, (un)substituted aryl; R2 = H, alkyl, etc.; R3, R4 = H, alkyl, halo, OH, alkoxy, etc.; X = OH, alkoxy, etc.; n = 0, 1, 2] were prepd. E.g., 2-[(2-phenylethyl)amino]thiophenol (prepn. given) was refluxed with 2-methoxy-4-isopropyl-7-formyl-2,4,6-cycloheptatrien-1-one in toluene for 17 H to give I [X = MeO, R1 = 5'-iso-Pr, R2 = PhCH2CH2, R3 = R4 = H, n = 0]. At 0.1 mg/Kg i.p. this showed 50% effectiveness in counteracting brain ischemic rats in a learning study using rats.

IT 142224-26-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, as intermediate for benzothiazolinyltropolones for treatment of ischemia)

RN 142224-26-8 HCAPLUS

CN 2(3H)-Benzothiazolone, 3-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing  
References

ACCESSION NUMBER:

1992:531223 HCAPLUS

DOCUMENT NUMBER:

117:131223

TITLE:

Preparation of heterocycltropolones as ischemia inhibitors

INVENTOR(S):

Ito, Noriie; Kuniyara, Mineo; Kushida, Hiroshi;  
McWhoster, William W.; Nomura, Syunji; Ozawa,  
Kazunori; Taniguchi, Mikeo; Tsuzuki, Tazuo

PATENT ASSIGNEE(S):

USA

SOURCE: PCT Int. Appl., 77 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

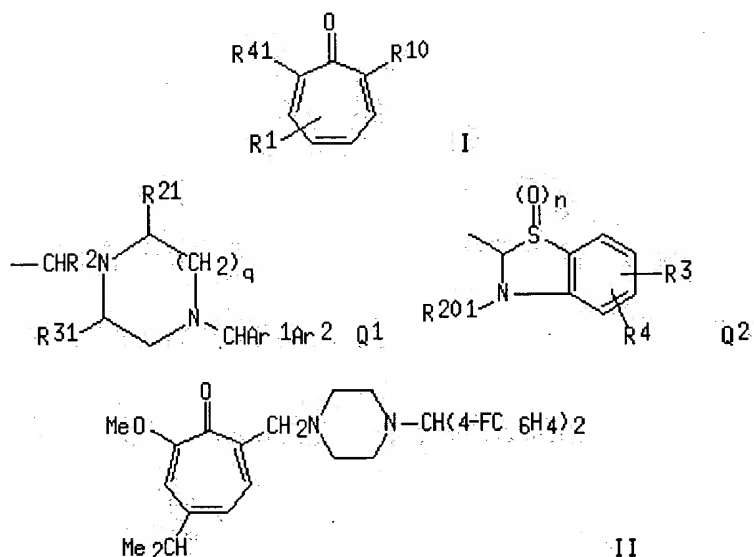
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9204338	A1	19920319	WO 1991-US5906	19910827
W: AU, BB, BG, BR, CA, CS, FI, HU, JP, KP, KR, LK, MC, MG, MN, MW, NO, PL, RO, SD, SU, US				
RW: AT, BE, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GN, GR, IT, LU, ML, MR, NL, SE, SN				
JP 04120069	A2	19920421	JP 1990-229536	19900829
AU 9187203	A1	19920330	AU 1991-87203	19910827
AU 651629	B2	19940728		
EP 546102	A1	19930616	EP 1991-917948	19910827
EP 546102	B1	19971015		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
HU 65943	A2	19940829	HU 1993-533	19910827
JP 06509318	T2	19941020	JP 1991-516629	19910827
JP 2512656	B2	19960703		
NO 9300669	A	19930225	NO 1993-669	19930225

## PRIORITY APPLN. INFO.:

JP 1990-229536	19900829
JP 1991-56252	19910131
JP 1991-39173	19910208
WO 1991-US5906	19910827

OTHER SOURCE(S): MARPAT 117:131223

GI



AB Title compds. I [R<sub>10</sub> = Q<sub>1</sub>, Q<sub>2</sub>; R<sub>1</sub>, R<sub>2</sub> = H, C1-5 alkyl, (substituted) aryl, (substituted) heterocyclyl; R<sub>3</sub>, R<sub>4</sub> = H, (substituted) C1-5 alkyl, C7-20 aralkyl, C7-20 aralkyl contg. O, S, or N atoms; halo, OH, C1-5 alkoxy, cyano, etc.; R<sub>41</sub> = OR<sub>3</sub>, OR<sub>6</sub>, NR<sub>7</sub>R<sub>8</sub>, etc.; R<sub>6</sub> = H, (substituted) C1-5 alkyl, etc.; R<sub>7</sub>, R<sub>8</sub> = H, (substituted) C1-5 alkyl, C7-20 aralkyl which may contain O, S, or N atoms; NR<sub>7</sub>R<sub>8</sub> = 5-7 membered ring which may contain

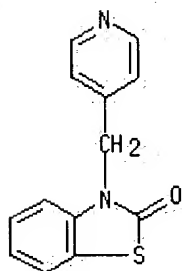
addnl. O or N atoms; R21, R31 = H, C1-3 alkyl; R201 = H, C1-5 alkyl, C2-20 aralkyl, C6-10 arylsulfonyl, C6-10 arylsulfonyl contg. O, S, or N atoms; Ar1, Ar2 = (substituted) aryl; n = 0-2; q = 1-2], were prepd. Thus, a soln. of 7-chloromethyl-4-isopropyl-2-methoxy-4-isopropyl-2,4,6-cycloheptatrien-1-one (prepn. given), 1-(4,4'-difluorobenzhydryl)piperazine, and Et3N in CHCl3 was refluxed for 20 h to give title compd. II. II had minimal ED of <5 mg/kg i.v. in a ischemic heart/reperfusion test in rats.

IT 142224-26-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, as intermediate for ischemia inhibitors)

RN 142224-26-8 HCAPLUS

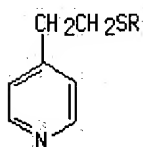
CN 2(3H)-Benzothiazolone, 3-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



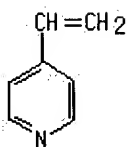
L4 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 1987:84351 HCAPLUS  
DOCUMENT NUMBER: 106:84351  
TITLE: 2-(4-Pyridyl)ethyl as a protective group for sulfur functionality  
AUTHOR(S): Katritzky, Alan R.; Takahashi, Ichiro; Marson, Charles M.  
CORPORATE SOURCE: Dep. Chem., Univ. Florida, Gainesville, FL, 32611, USA  
SOURCE: Journal of Organic Chemistry (1986), 51(25), 4914-20  
CODEN: JOCEAH; ISSN: 0022-3263  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 106:84351  
GI



I



II

AB 2-(4-Pyridyl)ethyl sulfides I (R = octyl, 2-naphthyl, Ph) were prepd. by Michael addn. of 4-vinylpyridine (II) with thiols RSH, whereas I [R = 5-nitro-2-pyridyl, CH2Ph, Bu, Bz, (PhS)CO] were prepd. by alkylation of thiol I (R = H) with RX (X = halide). I (R = CH2Ph) was also prepd. by alkylation of PhCH2SH with halide I (R = Cl). These sulfides and their corresponding sulfoxides and sulfones were depyridylethylated by quaternization and subsequent treatment with mild base to give the corresponding thiols, sulfinic acids, sulfonic acids, and sulfenamides. During one of these protection-deprotection sequences, Me 1-octyl sulfoxide was readily converted by aerial oxidn. into the corresponding

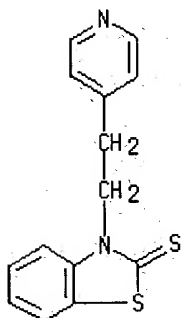
sulfone.

IT 27410-87-3

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with vinylpyridine)

RN 27410-87-3 HCAPLUS

CN 2(3H)-Benzothiazolethione, 3-[2-(4-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER:

1971:87880 HCAPLUS

DOCUMENT NUMBER:

74:87880

TITLE:

Michael and Mannich reactions with  
benzothiazole-2-thiol

AUTHOR(S):

Halasa, Adel F.; Smith, George E. P., Jr.

CORPORATE SOURCE:

Cent. Res. Lab., Firestone Tire and Rubber Co., Akron,  
OH, USA

SOURCE:

Journal of Organic Chemistry (1971), 36(5), 636-41  
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE:

Journal

LANGUAGE:

English

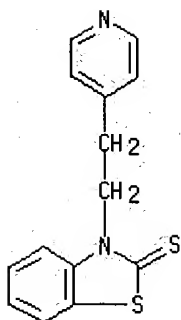
AB The reaction of the anion of benzothiazole-2-thiol (MBT) with activated olefins in the presence of NaH with Michael reaction acceptors produced 3-substituted benzothiazoline-2-thiones. Similarly, the Mannich reaction of MBT anion with HCHO and primary or secondary amines produced the N- (or 3-) substituted benzothiazoline-2-thiones. Possible mechanisms and supporting NMR, ir, and uv data are discussed. The N substitution of MBT anion is discussed within the framework of the oxibase scale which can predict the condition for formation of N products or S products from this ambident anion.

IT 27410-87-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 27410-87-3 HCAPLUS

CN 2(3H)-Benzothiazolethione, 3-[2-(4-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
--------------	----------------------

ACCESSION NUMBER: 1971:53769 HCAPLUS  
 DOCUMENT NUMBER: 74:53769  
 TITLE: 3-Substituted-2-benzothiazolinethiones  
 INVENTOR(S): Halasa, Adel F.  
 PATENT ASSIGNEE(S): Firestone Tire and Rubber Co.  
 SOURCE: U.S., 3 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3538109	A	19701103	US 1967-655761	19670725
PRIORITY APPLN. INFO.:			US 1967-655761	19670725

GI For diagram(s), see printed CA Issue.

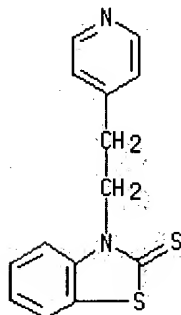
AB The title compds. (I) are all delayed-action rubber accelerators produced by Michael addns. to benzothiazoline-2-thione (II). Thus, II in freshly distd. THF stirred 48 hr with 4-vinylpyridine and NaH gave I (X = H, Y = 4-pyridyl), m. 159-61°. The corresponding I (X = H, Y = 2-pyridyl), m. 94-5° (alc.), was produced similarly. Analogous reaction of EtCH(NO<sub>2</sub>)CH<sub>2</sub>OAc with II give I (X = NO<sub>2</sub>, Y = Et), m. 89-90°. Similar Michael condensation of BzCH<sub>2</sub>CH<sub>2</sub>Cl with II yielded I (X = H, Y = Bz), m. 144.5-5.0° (CHCl<sub>3</sub>-EtOH).

IT 27410-87-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 27410-87-3 HCAPLUS

CN 2(3H)-Benzothiazolethione, 3-[2-(4-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)



=&gt; file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	45.13	202.44
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-5.54	-5.54

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=&gt; d his

(FILE 'HOME' ENTERED AT 15:22:35 ON 09 APR 2004)

FILE 'REGISTRY' ENTERED AT 15:22:40 ON 09 APR 2004

L1 STRUCTURE UPLOADED  
 L2 2 S L1  
 L3 45 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 15:25:39 ON 09 APR 2004

L4 7 S L3  
 L5 1 S L4 AND ROCHER, J?/AU  
 L6 1 S L4 AND YAMABE, H?/AU  
 L7 0 S L6 NOT L5  
 L8 1 S L4 AND CHAKI, H?/AU  
 L9 0 S L8 NOT L6  
 L10 1 S L4 AND ABE, M?/AU  
 L11 0 S L10 NOT L6  
 L12 1 S L4 AND OKUYAMA, M?/AU  
 L13 0 S L12 NOT L10

FILE 'CAOLD' ENTERED AT 15:27:42 ON 09 APR 2004

=&gt; s l3

L14 0 L3

=&gt; file beilstein

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.42	202.86

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-5.54

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FILE RELOADED ON OCTOBER 20, 2002  
 FILE LAST UPDATED ON MARCH 30, 2004

FILE COVERS 1771 TO 2003.  
**FILE CONTAINS 8,932,479 SUBSTANCES**

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 Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a molecular formula or a structure search for example can be restricted to compounds with available reaction information by concatenation with PRE/FA, REA/FA or more general with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be selected from substance answer sets and searched in the next step as reaction partner BRNs - Reactant (RX.RBRN) or Product BRN (RX.PBRN). After a search for reaction details substance documents associated with reactants or products may be retrieved by searching RX.PBRNs or RX.RBRNs as BRNs. <<<

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FILE 'REGISTRY' ENTERED AT 15:22:40 ON 09 APR 2004

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L3          45 S L1 FULL
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FILE 'HCAPLUS' ENTERED AT 15:25:39 ON 09 APR 2004

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L6          1 S L4 AND YAMABE, H?/AU
L7          0 S L6 NOT L5
L8          1 S L4 AND CHAKI, H?/AU
L9          0 S L8 NOT L6
L10         1 S L4 AND ABE, M?/AU
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 L12 1 S L4 AND OKUYAMA, M?/AU  
 L13 0 S L12 NOT L10

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FILE 'BEILSTEIN' ENTERED AT 15:27:52 ON 09 APR 2004

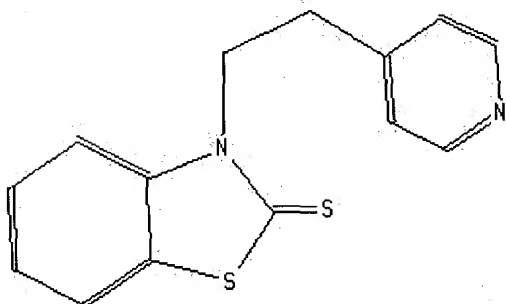
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L15 1 L3

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L15 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 1217129  
 Beilstein Pref. RN (BPR): 27410-87-3  
 CAS Reg. No. (RN): 27410-87-3  
 Chemical Name (CN): 3-(2-pyridin-4-yl-ethyl)-3H-benzothiazole-2-thione  
 Autonom Name (AUN): 3-(2-pyridin-4-yl-ethyl)-3H-benzothiazole-2-thione  
 Molec. Formula (MF): C14 H12 N2 S2  
 Molecular Weight (MW): 272.38  
 Lawson Number (LN): 31156, 27396  
 Compound Type (CTYPE): heterocyclic  
 Constitution ID (CONSID): 1157666  
 Tautomer ID (TAUTID): 1192884  
 Beilstein Citation (BSO): 5-27, 6-27  
 Entry Date (DED): 1988/11/29  
 Update Date (DUPD): 1993/02/15



Field Availability:

Code	Name	Occurrence
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BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2

CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	2
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	2
MP	Melting Point	4
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	4
UVS	UV and Visible Spectrum	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	3
RXPRO	Substance is Reaction Product	3

=> fil reg; d acc 27410-87-3; fil BEILSTEIN

FILE 'REGISTRY' ENTERED AT 15:28:21 ON 09 APR 2004

ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 27410-87-3 REGISTRY

CN 2(3H)-Benzothiazolethione, 3-[2-(4-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

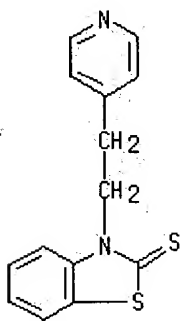
CN 2-Benzothiazolinethione, 3-[2-(4-pyridyl)ethyl]- (8CI)

FS 3D CONCORD

MF C14 H12 N2 S2

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, CHEMCATS, IFICDB, IFIPAT, IFIUDB

(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

FILE 'BEILSTEIN' ENTERED AT 15:28:21 ON 09 APR 2004

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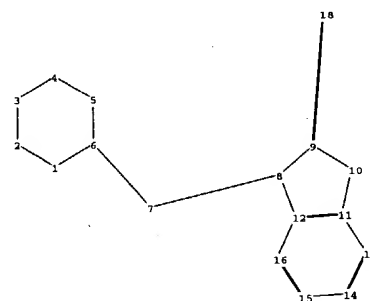
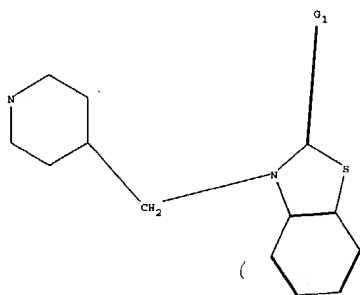
FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
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0.00	-5.54

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STN INTERNATIONAL LOGOFF AT 15:28:27 ON 09 APR 2004



chain nodes :

7 18

ring nodes :

1 2 3 4 5 6 8 9 10 11 12 13 14 15 16

chain bonds :

6-7 7-8 9-18

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12 11-13 12-16 13-14 14-15 15-16

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-18

exact bonds :

6-7 7-8 9-10 10-11

normalized bonds :

11-12 11-13 12-16 13-14 14-15 15-16

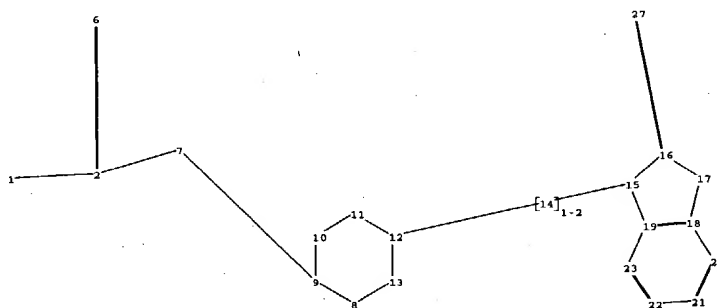
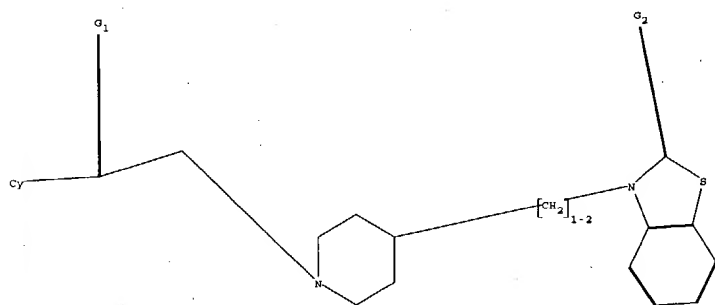
isolated ring systems :

containing 1 : 8 :

G1:O,S

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 18:CLASS



chain nodes :

1 2 3 6 7 14 27

ring nodes :

8 9 10 11 12 13 15 16 17 18 19 20 21 22 23

chain bonds :

1-2 2-6 2-7 7-9 12-14 14-15 16-27

ring bonds :

8-9 8-13 9-10 10-11 11-12 12-13 15-16 15-19 16-17 17-18 18-19 18-20 19-23  
20-21 21-22 22-23

exact/norm bonds :

1-2 2-6 7-9 8-9 8-13 9-10 10-11 11-12 12-13 15-16 15-19 16-27

exact bonds :

2-7 12-14 14-15 16-17 17-18

normalized bonds :

18-19 18-20 19-23 20-21 21-22 22-23

isolated ring systems :

containing 8 : 15 :

G1:O,[\*1]

G2:O,S

Match level :

1:Atom 2:CLASS 3:CLASS 6:CLASS 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom  
13:Atom 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom  
23:Atom 27:CLASS

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 NEWS 3 NOV 24 MSDS-CCOHS file reloaded  
 NEWS 4 DEC 08 CABA reloaded with left truncation  
 NEWS 5 DEC 08 IMS file names changed  
 NEWS 6 DEC 17 DGENE: Two new display fields added  
 NEWS 7 DEC 18 BIOTECHNO no longer updated  
 NEWS 8 DEC 19 CROPU no longer updated; subscriber discount no longer available  
 NEWS 9 DEC 22 ABI-INFORM now available on STN  
 NEWS 10 JAN 27 Source of Registration (SR) information in REGISTRY updated and searchable  
 NEWS 11 JAN 27 A new search aid, the Company Name Thesaurus, available in CA/CAPLUS  
 NEWS 12 FEB 05 German (DE) application and patent publication number format changes  
 NEWS 13 MAR 03 MEDLINE and LMEADLINE reloaded  
 NEWS 14 MAR 03 MEDLINE file segment of TOXCENTER reloaded  
 NEWS 15 MAR 03 FRANCEPAT now available on STN  
 NEWS 16 MAR 29 Pharmaceutical Substances (PS) now available on STN  
 NEWS 17 MAR 29 WPIFV now available on STN  
 NEWS 18 MAR 29 No connect hour charges in WPIFV until May 1, 2004  
 NEWS 19 MAR 29 New monthly current-awareness alert (SDI) frequency in RAPRA

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 MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
 AND CURRENT DISCOVER FILE IS DATED 3 MARCH 2004  
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FULL ESTIMATED COST	0.21	0.21

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 DICTIONARY FILE UPDATES: 7 APR 2004 HIGHEST RN 672883-15-7

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<http://www.cas.org/ONLINE/DBSS/registryss.html>

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L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

=> s l1

SAMPLE SEARCH INITIATED 14:13:31 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS 1 ANSWERS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 2 TO 124  
 PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS  
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
 FULL SEARCH INITIATED 14:13:35 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 44 TO ITERATE

100.0% PROCESSED 44 ITERATIONS 18 ANSWERS  
 SEARCH TIME: 00.00.01

L3 18 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	156.26	156.47

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FILE COVERS 1907 - 9 Apr 2004 VOL 140 ISS 16  
FILE LAST UPDATED: 8 Apr 2004 (20040408/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L4 1 L3

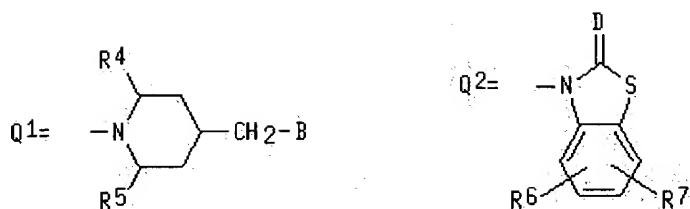
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L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing  
Text References

ACCESSION NUMBER: 1999:311193 HCAPLUS  
DOCUMENT NUMBER: 130:338102  
TITLE: Preparation of N-(aminoalkyl)- or N-(1-piperidinylmethyl)benzothiazoline derivatives as ligands for sigma-receptor  
INVENTOR(S): Rocher, Jean-Philippe; Yamabe, Haruko; Chaki, Haruyuki; Saito, Ken-ichi; Abe, Michikazu; Okuyama, Masahiro  
PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan  
SOURCE: PCT Int. Appl., 95 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9923083	A1	19990514	WO 1998-JP4973	19981104
W: CA, CN, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1043319	A1	20001011	EP 1998-951687	19981104
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 11217377	A2	19990810	JP 1998-314459	19981105
PRIORITY APPLN. INFO.:			JP 1997-302607	A 19971105
			WO 1998-JP4973	W 19981104
OTHER SOURCE(S):		MARPAT 130:338102		
GI				



AB Compds. represented by the following formula, such as (R,S)-1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol, or salts thereof: X-Q-C(R1)(R2)-Z [wherein R1 and R2 each represents hydrogen, alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; and Z represents either of groups NR3(CH2)p and Q1; wherein R3 represents alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; p is an integer of 3 to 8; R4 and R5 each represents hydrogen or alkyl or they together with other interposing atoms represent a 5- to 7-membered heterocyclic ring; and B represents formula Q2 (wherein R6 and R7 each represents hydrogen, halogeno, NO2, alkyl, cycloalkyl, alkenyl, haloalkyl, OH, alkoxy, haloalkoxy, alkoxycarbonyl, Ph, (un)substituted NH2, alkylthio, etc.); D represents sulfur, oxygen, or (un)substituted NH; when X represents optionally alkyl-substituted mono- or polycyclic alkyl, cycloalkylalkyl, aryl, or heteroaryl, Q represents CO, C(:NOH), C(Y)(A) (wherein Y represents H, alkyl, alkenyl, alkynyl, etc. and A represent OH, alkoxy, cycloalkoxy, cycloalkylalkoxy, alkenyloxy, aryloxy, etc.); or when X represents a 8- to 10-membered bicyclic heteroaryl contg. 1 or 2 heteroatoms, Q represents single bond], which have high affinity to  $\sigma$ -receptors and exhibit small inhibition consts.  $K_i$  against  $\sigma$ -1 and/or  $\sigma$ -2 receptors, are prepd. Also claimed are therapeutics contg. I as the active ingredients for the treatment and/or prevention of diseases caused or enhanced by nerve-regulating effect of  $\sigma$ -ligands. They are useful for the treatment and/or prevention of central nervous system diseases, intestinal diseases, and cardiovascular diseases. Thus, 4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidine was condensed with 1-(bromoacetyl)adamantane in the presence of K2CO3 followed by NaBH4 redn. in ethanol and THF and acidification with HCl in EtOAc to give 1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol hydrochloride (II). II and 3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-5-chloro-2-oxobenzothiazoline hydrochloride inhibited the binding of [H3]-di-o-tolylguanidine to  $\sigma$ -receptor (P2 membrane fraction) prepn. from rat liver with  $K_i$  value of 7.0 and 3.1 nM, resp., as compared to  $K_i$  of 29 nM for haloperidol. A tablet, an injection, and an ointment formulation contg. II were described.

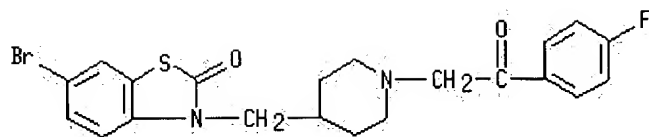
IT **224443-05-4P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of N-(aminoalkyl)- or N-(1-piperidinyl)benzothiazoline derivs. having high affinity to sigma-receptor as therapeutics)

RN 224443-05-4 HCAPLUS

CN 2(3H)-Benzothiazolone, 6-bromo-3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



# HCl

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

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FILE 'REGISTRY' ENTERED AT 14:11:48 ON 09 APR 2004

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 18 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 14:13:38 ON 09 APR 2004

L4 1 S L3

FILE 'CAOLD' ENTERED AT 14:13:48 ON 09 APR 2004

=&gt; s 13

L5 0 L3

=&gt; file beilstein

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 FILE LAST UPDATED ON MARCH 30,2004

FILE COVERS 1771 TO 2003.

**FILE CONTAINS 8,932,479 SUBSTANCES**

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 Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a molecular formula or a structure search for example can be restricted to compounds with available reaction information by concatenation with PRE/FA, REA/FA or more general with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be selected from substance answer sets and searched in the next step as reaction partner BRNs - Reactant (RX.RBRN) or Product BRN (RX.PBRN). After a search for reaction details substance documents associated with reactants or products may be retrieved by searching RX.PBRNs or RX.RBRNs as BRNs. <<<

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 L6 0 L3

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